# Fermion Monte Carlo Calculations on BlueGene/L

**Malvin H. Kalos**

**Lawrence Livermore National Laboratory**
**Livermore, CA 94550 USA**

**BlueGene/L Workshop**
**Lake Tahoe, Nevada**
**August 14, 2002**

# Aim

**To develop a method for many-fermion systems that is efficient in Monte Carlo sense and polynomial in particle number**

**And with no uncontrolled approximations**

# Computational demands

- Population of random walkers divided into distributed memory
- Drift, diffuse and branch walkers in each processor
- Population balanced across distributed memory
- Process iterated
- Ideally suited for BlueGene/L
- Memory Requirements, $\gtrsim$ 5 Megabytes/processor
- Active Data, $\gtrsim$ 2.5 Megabytes/processor
- Don’t yet know how complexity grows with particle number except not N!
- Previous pitfalls that lead to exponential growth are avoided

# Research aims

- Understand and optimize method for:
  - Atoms
  - Molecules
  - Nuclear physics
  - Extensive systems
- Apply to significant problems in physics and chemistry
  - Extend to temperature > 0
  - Apply to hydrogenic systems
- Development, experiments and production demand very high performance computing

# Diffusion Monte Carlo

**Diffusion Monte Carlo solves Schrodinger Equation in Imaginary time.**

**But how can Monte Carlo get "chemical accuracy," about $10^{-5}$ relative error in eigenvalue.**

**Importance sampling:**

**Construct random walk for** $y_G(R)y(R)$

**Where** $y_G(R)$ **is a "guiding function," ideally equal to exact solution, but approximation is OK.**

# Importance Sampled Diffusion

**Random walk is a Langevin process with branching**

$$\vec{R} \rightarrow \vec{R} + dt\ \vec{\nabla} y_G$$

$$\vec{R} \rightarrow \vec{R} + \sqrt{dt}\ \vec{U}; \quad \vec{U} \text{ a vector of NRV's with mean O, variance 1}$$

$$\langle M \rangle = exp\left[ +dt\left( E_T - \frac{Hy_G}{y_G}\bigg|_R \right) \right]$$

**Finds fundamental modes very quickly and efficiently in many dimensions.**

**Fermions require solutions not everywhere positive!**

**What to do?**

# Fixed-Node Application

**Standard: impose non-physical boundary condition that** $y = 0$ ***when*** $y_G = 0$

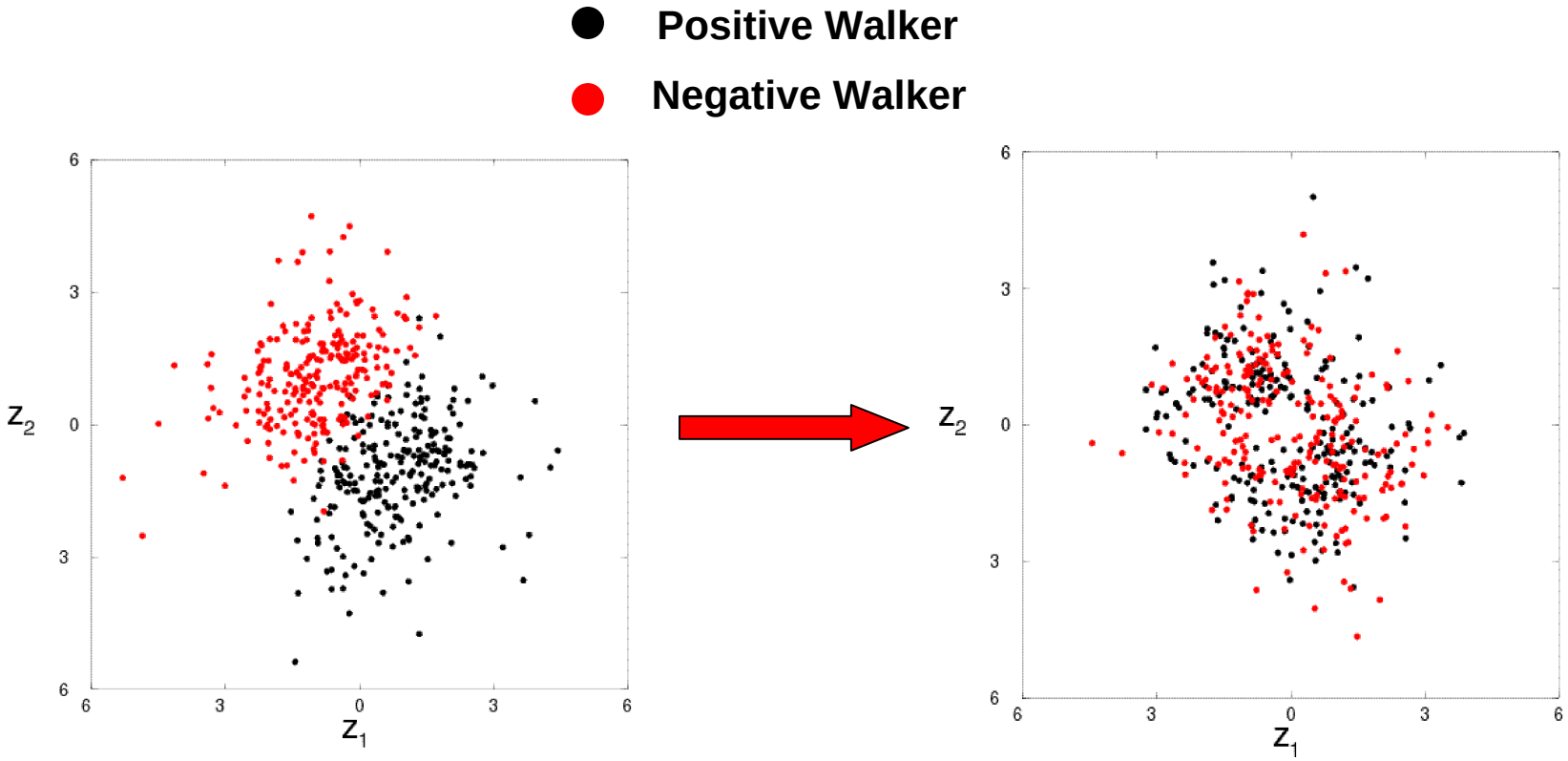
**This is an uncontrolled approximation!**

**How to do better?**

**Use walkers that carry signs**

**By itself, this device accomplishes nothing**

# $H_2$ molecule



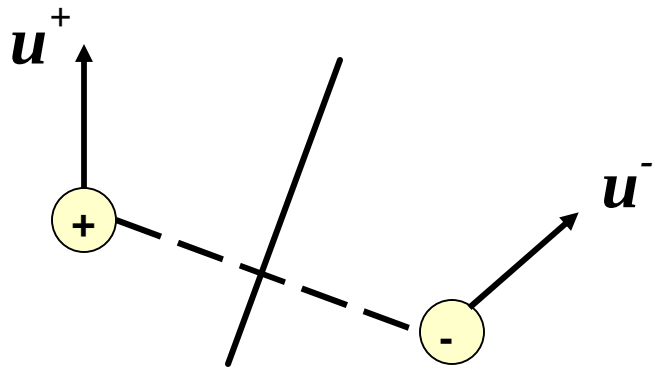

**Released-node DMC with signed walkers unstable**

# Ingredients for stability

1) Distinct positive guiding functions for positive and negative walkers

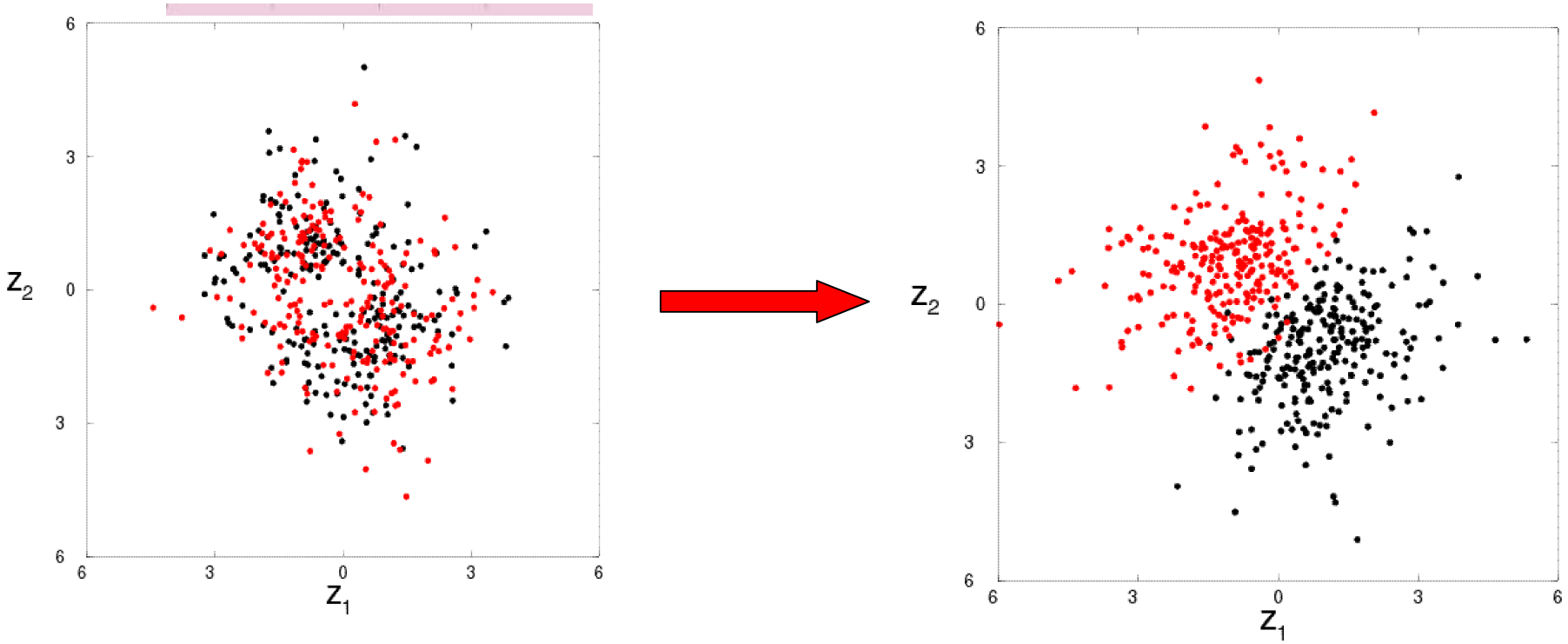
$$\Psi_G^{\pm}(\boldsymbol{R}) = \sqrt{\Psi_S^2(\boldsymbol{R}) + c^2\Psi_A^2(\boldsymbol{R})} \pm c\Psi_A(\boldsymbol{R})$$

2) Positive and negative walkers paired with correlated diffusion




3) Cancellation between positive and negative walkers with expected future contributions conserved

# $H_2$ molecule




**With three ingredients DMC is stable**

# Other Systems Studied

- He atom
- Be atom

  - 14 He atoms in periodic system
  - 7 Free Fermions in periodic system
  - 19 Free Fermions in periodic system
  - 27 Free Fermions in periodic system

  } PRL 85 3547 (2000)

- In progress
  - 54 He atoms in periodic system
  - $Li_2$ molecule
  - $Be_2$ molecule
  - $B_2$ molecule
  - Two-dimensional electron gas